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Probing Interfacial Momentum Closures in Two-Phase Bubbly Flow with Machine Learning-Aided Methods

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INTRODUCTION

Computational fluid dynamics (CFD) approach has already reached a high level of maturity for single-phase flows, however the development of closure models for two-phase flow requires additional attention. Multiphase CFD (M-CFD) methods resolve the conservation equations for mass, momentum and energy while differing in the approaches and strategies adopted in the physical closure models. The most widely adopted framework for M-CFD is the Eulerian-Eulerian two-fluid approach which assumes that all phases are co-existing inside each computational cell. For each fluid, the full set of conservation equations is solved; therefore, each fluid has a different velocity field. For adiabatic two-phase flow, the mechanisms of the interfacial momentum transfer are modeled by the interfacial forces representing different physical mechanisms. One of the crucial issues in the development and application of two-fluid model is the understanding of the interfacial momentum closures which determines the bubble distribution and migration behaviors. Dedicated experiments [1] are performed to support the physical understanding and drive the closures' development [1-4]. However, limitations exist due to the uncertainties in the experimental measurement and the simplified analytical assumptions [5] which have difficulties on representing the complex non-linear flow fields.

In this paper, a data-driven approach, Feature Similarity Measurement (FSM), is developed and proposed to resolve the challenges of modeling the interfacial forces closures. Case study is performed with two-phase flow scenarios where the high-fidelity experimental data is available. Within the Eulerian-Eulerian two-fluid framework, only momentum equations for gas and liquid phases are solved and reduced-order interfacial momentum closures are aided with FSM. Predictions of void fraction and velocity fields are analyzed and demonstrate the potential of machine learning-driven interfacial forces closures.

FEATURE SIMILARITY MEASUREMENT

Feature Similarity Measurement (FSM), developed by Bao [6-9], integrates model error, mesh-induced error and scaling uncertainty together, and estimates the simulation error by exploring local patterns in multi-scale data with the usage of deep learning. The underlying local patterns in multi-scale data are represented by a set of physical features, which are defined based on physical system of interest, empirical correlations and local mesh size. After generating an error database using high-fidelity (validated experimental/numerical data) and low-fidelity data (fast-running coarse-mesh simulation results), deep learning algorithms are applied to explore the relationship between the local physical features and local simulation errors to develop a surrogate model. The basic idea of FSM was proposed in [8] as shown in Fig. 1.

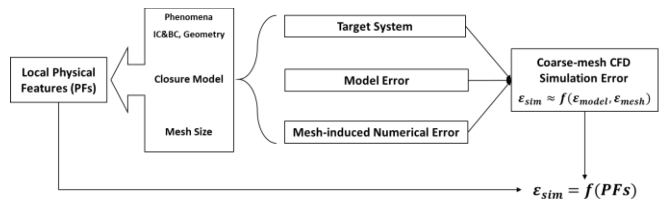

Fig. 1. Basic idea of FSM: identify the relationship between physical features and simulation error [8]

FSM includes following steps: identifying local physical features, measuring the similarity of local physical features, and investigating the relationship between physical feature similarity and machine learning prediction accuracy. For the applications of the FSM approach, a turbulent mixing case study was performed to evaluate the predictive capability of FSM for globally extrapolated conditions in [6]. A data-driven framework was developed to improve applications of the coarse-mesh codes by predicting their simulation errors and suggesting the optimal mesh size and closure models for system-level simulations based on the FSM approach [7]. In [8], FSM was improved as a data-driven guidance to improve the coarse-mesh CFD simulation capability for two-phase flow with a substantially reduced computational cost. In [9], FSM was applied for a 2D mixed convection problem considering turbulence. Case studies showed that FSM has good predictive capability. The prediction accuracy increases with the increasing of data similarity of physical features.

However, in all these applications, high-fidelity data was generated using validated fine-mesh CFD simulations. It's difficult to combine specific appropriate empirical closures and local mesh sizes to validate these "high-fidelity" CFD simulations. Particularly when the experimental data has large ranges for global conditions, such as largely different injection rates and void fraction for a pipe flow. There is no a set of closures that has the capability to accurately predict all different conditions. Therefore, this paper is proposed to directly use experimental data as high-fidelity data for correcting coarse-mesh low-fidelity simulations.

A Deep Feedforward Neural Network (DFNN) was trained using training datasets to predict the simulation errors of coarse-mesh low-fidelity simulations with high-fidelity data. By adding the predicted simulation errors to the original coarse-mesh low-fidelity simulation results, the DFNN-corrected results can be obtained and compared with the high-fidelity data.

CASE STUDY

In this paper, a case study based on two-phase flow was performed to evaluate the predictive capability of FSM. Four tests were designed using different high-fidelity and low-fidelity data. 42 reference experimental datasets are from Liu and Bankoff [10] and used as Type-I high-fidelity data. Type-II high-fidelity data was generated using the commercial CFD package, STAR-CCM+12.06, with 25-cell mesh configuration and following two-phase interfacial forces closures and turbulence models: drag force model from Tomiyama [2], lift correction from Shaver and Podowski [11] with a base coefficient of 0.025, turbulent dispersion force from Burns [12] and the standard *k-ε* turbulence model. The set of these models which is referred as the Bubbly and Moderate Void Fraction (BAMF) model has been tested for 12 cases from the Liu and Bankoff experimental datasets, which provided reasonable predictions for mean flow profiles of void fraction and phase velocities [4]. To accelerate the simulation, only one-quarter of the domain is simulated, and symmetric boundary conditions are applied on the two side surfaces. The cross-sectional view of the mesh configurations is shown in Fig. 2. Quantities of Interest (QoIs) in this case study are liquid and vapor velocities (u_l and u_g), and void fraction (α).

Low-fidelity data was also generated using STAR-CCM+ with three different coarse meshes, as shown in Fig.2. The number of cells from the wall to the pipe center ranges from 10 to 20. Mesh configuration is crucial to the accurate prediction of the multiphase flow phenomena using CFD approaches. The calculation of flow variables gradients depends on the mesh resolution between two adjacent cells which are directly relevant to certain physical models. For example, the lift force relies on the gradient of velocity and the magnitude of turbulence dispersion force depends on the gradient of void fraction. In addition, the near wall mesh resolution determines numerous closures near the wall, like velocity wall function. The lift coefficient model proposed by Shaver and Podowski [12] also depends on the ratio between wall distance and interaction length scale.

Type-I low-fidelity data was generated using BAMF model, while Type-II low-fidelity data was generated by solving basic momentum equations and standard two-equation $\kappa - \varepsilon$ turbulence model without BAMF closures.

For this case study, 26 physical features were identified according to the classification of physical features, as shown in Table I. 16 of these physical features are the 1-order and 2-order derivatives of key variables and other 10 physical features are the typical non-dimensional parameters defined based on the model parameters and mesh sizes. The goal of this case study is to answer two questions: (1). Is FSM able to improve the coarse-mesh low-fidelity simulations to reach the accuracy of high-fidelity data? (2). Does FSM work well for different types of low-fidelity and high-fidelity data?

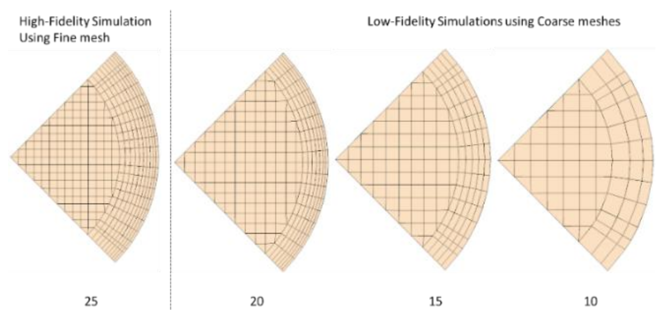

Fig. 2. Mesh configuration for high-fidelity and low-fidelity simulations using STAR-CCM+

TABLE I. List of selected physical features for the two-phase flow case study

Local Physical Features							
Derivatives of variable				Local physical parameters			
1-order		2-order		Non-dimensional groups		Parameters relevant to closure models, IC/BC, geometry	
$\frac{du_l}{dx}$	$\frac{du_g}{dx}$	$\frac{d^2u_l}{dx^2}$	$\frac{d^2u_g}{dx^2}$	$Re_\Delta = \frac{\rho_l \Delta \cdot \Delta u}{\mu_l}$	$I_l = \frac{k_l}{{u_l}^2}$	$R_l = \frac{{k_l}^{\frac{3}{2}}}{\varepsilon_l D_b}$	$R_\mu = \frac{\mu_g^t}{\mu_L^t}$
$\frac{d\alpha}{dx}$	$\frac{dP}{dx}$	$\frac{d^2\alpha}{dx^2}$	$\frac{d^2P}{dx^2}$	$Re_b = \frac{\rho_l D_b \Delta u}{\mu_l}$	$I_g = \frac{k_g}{{u_g}^2}$	$R_g = \frac{{k_g}^{\frac{3}{2}}}{\varepsilon_g D_b}$	$r_l = \frac{\mu_l^t}{\mu_l}$
$\frac{dk_l}{dx}$	$\frac{dk_g}{dx}$	$\frac{d^2k_l}{dx^2}$	$\frac{d^2k_g}{dx^2}$	$We = \frac{\rho D_b \Delta u^2}{\sigma}$		$Re_y = \frac{\rho_l y \Delta u}{\mu_l}$	$R_b = \frac{D_b}{\Delta}$
$\frac{d\varepsilon_l}{dx}$	$\frac{d\varepsilon_g}{dx}$	$\frac{d^2\varepsilon_l}{dx^2}$	$\frac{d^2\varepsilon_g}{dx^2}$				

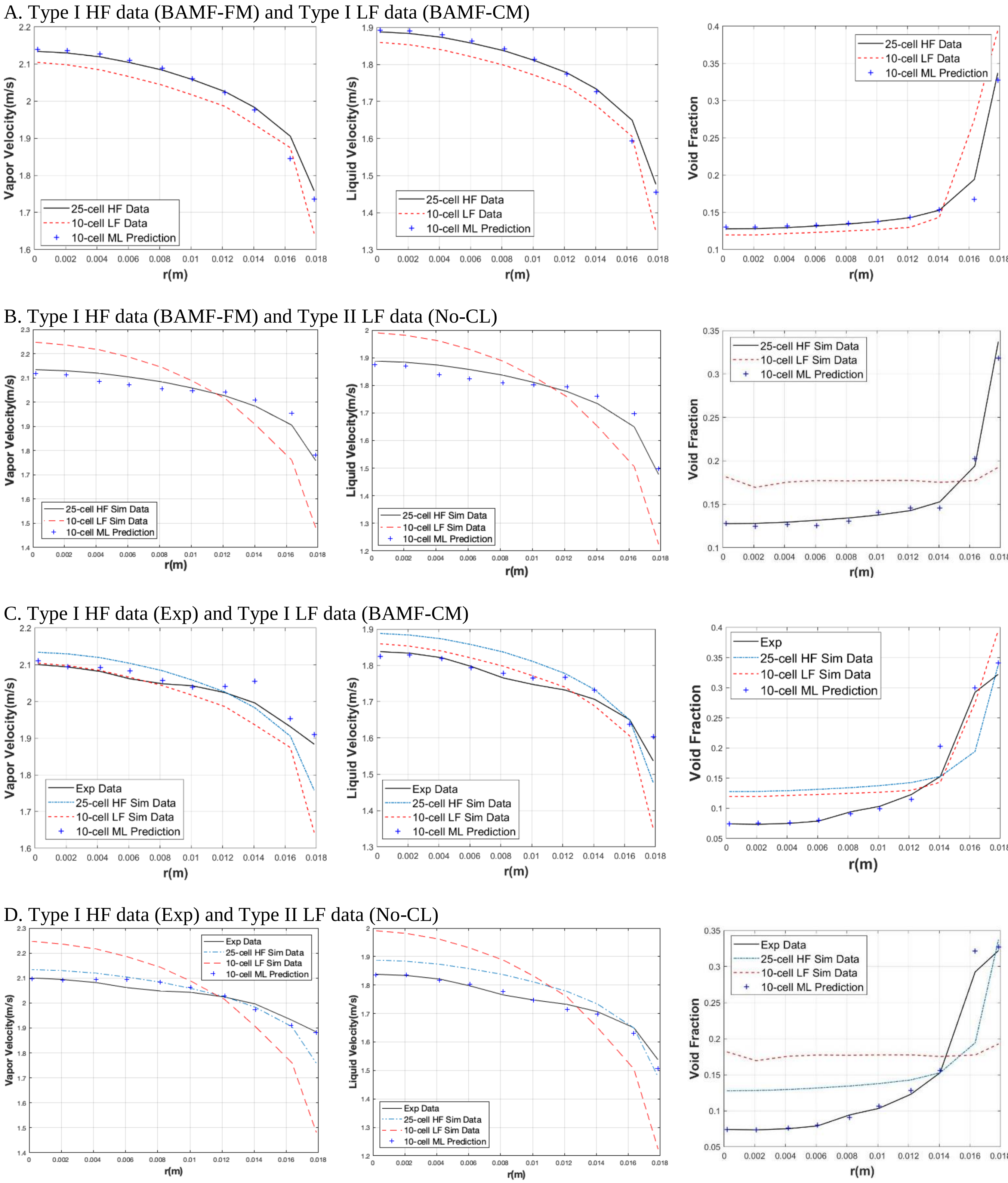

Fig. 3. Comparisons between DFNN predicted results and original low-fidelity simulation results of case 42 for 10-cell coarse mesh configuration (HF: high-fidelity, LF: low-fidelity, FM: fine-mesh, CM: coarse-mesh, Exp: experimental data, No-CL: without BAMF or other interfacial closures, Sim: simulation, ML: machine learning)

All the 42 cases have different values for void fraction and phase velocities. Case 42 with highest injection rates and highest void fraction was selected as testing case while all other cases were used for generating training database. Training data was used for the training of a DFNN model to predict the errors of coarse-mesh low-fidelity simulations compared to high-fidelity data. For two types of high-fidelity and low-fidelity data, Fig. 3 represents the DFNN predictions for four tests with different datasets. It shows that no matter which type of high-fidelity or low-fidelity data is used, FSM has the capability to capture their differences and correct low-fidelity data to the selected high-fidelity data. Effects of Model-induced error and physical model error are considered and reduced simultaneously. DFNN predictions are closer to high-fidelity data than original low-fidelity data. Without the DFNN corrections, the original coarse-mesh low-fidelity results show different patterns with the high-fidelity data, especially for void fraction in No-CL condition. As expected, a flat void fraction profile is predicted in the No-CL low-fidelity simulations because no interfacial closures are selected for the transverse direction.

After the training, the DFNN model well captures this flat pattern and provides an appropriate correction to match the high-fidelity results. The capability of capturing regional patterns results from identifying 1-oder and 2-order derivatives of QoIs as the physical features, because not only the characteristic at this point are captured, but also the connections of this point with its neighboring points. Low-fidelity simulations were greatly improved after FSM-aided corrections.

CONCLUSICON

This paper demonstrated a data-driven approach Feature Similarity Measurement (FSM) for the error estimation in two-phase flow simulations using coarse-mesh CFD to achieve a comparable accuracy as experimental data or fine-mesh simulation results. Uncertainty of coarse-mesh low-fidelity simulations can be reduced by learning from high-fidelity data using FSM. In this work, the prediction performance, fast-running capability and scalability of the FSM approach has been demonstrated upon a two-phase flow case study. The original coarse-mesh simulation results were greatly improved by being corrected by the well-trained DFNN models for global extrapolative conditions.

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